# Morphology and stability of the C/BN and SiC/GaN interfaces based on *ab initio studies*

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Excellent physical properties of boron nitride (c-BN, h-BN) are crucial for technological development of micro-, or nanoelectronic devices, high-temperature ceramic applications, protective coatings, and optoelectronic devices operating in the visible/ultra-violet range [1-3]. The C/BN heterostructures are of importance for these applications, as well as the knowledge on the microscopic details of interfaces' morphology and stability.

In this report, we discuss diamond/BN and 3C-SiC/GaN heterostructure junctions as a prototype of the interfaces between B/C, N/C, Ga/C, Ga/Si and N/Si atomic layers. Our studies are based on *ab-initio* DFT calculations. In the studied heterostructures, we concentrate on the two important growth directions, i.e., [001] and [111] ones. In both cubic directions the abrupt C/N and C/B interfaces contain 'oversaturated' or 'undersaturated' tetrahedral bonds [4]. Such bond heteropolarity results in macroscopically charged interfaces that are mostly energetically unstable and should undergo various reconstructions [4]. We propose some reconstruction patterns, which involve substitution of certain number of either III- or V-valency atoms by carbon atoms in the epitaxially grown BN monolayers, as well as one mixed atomic layer (N/C or B/C), depending on the crystallographic orientation. We employ both a slab and the non-stoichiometric super-lattice approaches by creating super-cells having up to 104 atoms, with lateral 2x2 unit cell. The computations of the total energies of the abrupt and reconstructed interfaces, and laterally averaged distributions of the total potential and charge enabled to find the preferred bonding configurations, as well as the resulting valence electron charge densities in the systems studied. Comparison of the obtained results in the slab approach for C/c-BN, interfaces in the [111] direction with the respective ones for the crystallographically equivalent 3C-SiC/GaN interfaces shows the preferred reconstructed C-Ga(B) interface type. The energy gain resulting from the charge compensation by C atoms mixed in III-valency atom layer is up to 2.8 eV/atom. The computed formation enthalpies, valence band offsets (VBO's), induced interface charges, and electric fields provide microscopic knowledge about C/nitride and SiC/nitride interface morphology.

Finally, we investigate the role of van der Waals interaction between the graphene monolayer on h-BN and c-BN in the inter-planar binding energy.

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